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Input to the NSF Study on Computational Requirements in Geosciences

T. Antoun, I. Lomov, J. Morris

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Tarabay Antoun, Ilya Lomov, Joseph Morris
Computational Physics Group
Earth Sciences Division
Lawrence Livermore National Laboratory

The Computational Physics Group of the Earth Sciences Division focuses much of its effort on improving current understanding of the response of geologic media to strong shock waves, and on the interaction of those waves with underground structures. Two codes have been developed and used to achieve these objectives: LDEC and GEODYN. Both codes are three-dimensional and massively parallel, and they have both been used on LLNLs high performance computing platforms to advance the state of the art in computational geophysics.

Propagation of Shock Waves in Geologic Media

Geologic media are multi-layered, with different layers having different shock wave propagation characteristics. Faults and discontinuities often intersect the layers, thus rendering most geologic settings three-dimensional for the purpose of wave propagation simulations. Among the parameters of interest in shock wave propagation problems are peak stress, and peak particle velocity, and resolving them requires small cell size at the shock front. Additionally, problems of interest usually involve propagation distances of hundreds of meters. The three-dimensional nature of the problem, coupled with the requirements for high resolution and long propagation distance lead to simulations that are too large for single processor computers, and impractically large for large-scale computers. A recently performed 3D simulation of the Baneberry underground nuclear test is described below as an illustrative example. Limitations in problem size coupled with memory and storage requirements make it practically impossible to routinely perform 3D simulations like this without dedicated access to significant resources on the largest and most modern platforms currently available.

Baneberry, a 10-kiloton nuclear event, was detonated at a depth of 278 m at the Nevada Test Site on December 18, 1970. Shortly after detonation, radioactive gases emanating from the cavity were released into the atmosphere through a shock-induced fissure near surface ground zero. Extensive geophysical investigations, coupled with a series of 1D and 2D computational studies were used to reconstruct the sequence of events that led to the catastrophic failure. However, the geological profile of the Baneberry site is complex and inherently three-dimensional, which meant that some geological features had to be simplified or ignored in the 2D simulations. This left open the possibility that features unaccounted for in the 2D simulations could have had an important influence on the eventual containment failure of the Baneberry event.

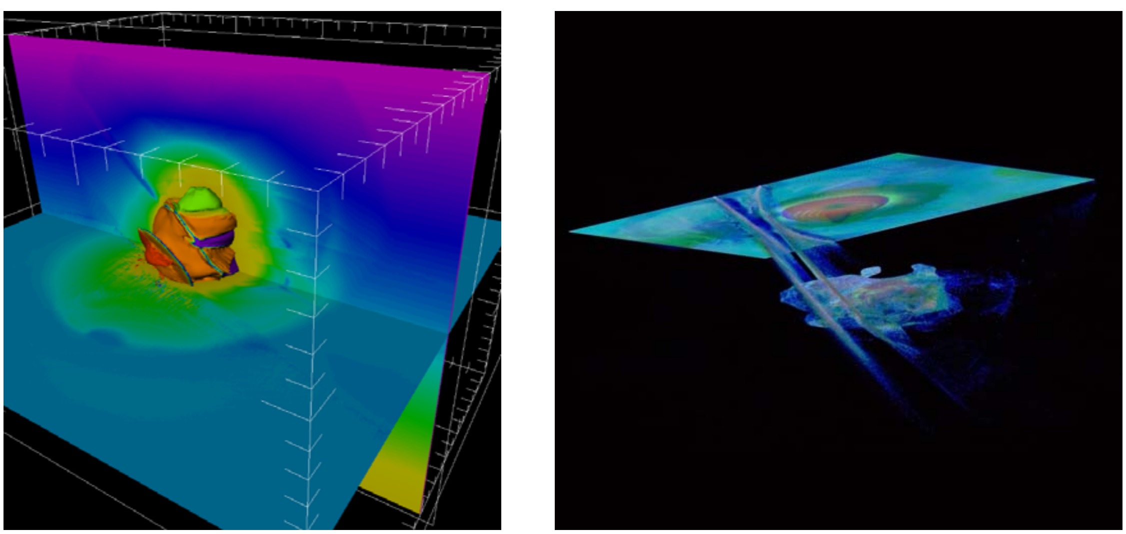
To address this issue, a new study was undertaken [1]. The study encompassed 3D high fidelity simulations based on the most accurate geologic and geophysical data available. The simulations were performed in GEODYN, a Eulerian Godunov code with adaptive mesh refinement. GEODYN has been used to simulate problems involving the interaction of shock waves with geologic media. Among its features, the code includes high-order interface reconstruction, and advanced constitutive models that incorporate many phenomenological features of the dynamic response of geologic media. The simulation included ~40 million zones, and required ~40000 CPU hours to complete, thus making it the largest simulation of its kind. The simulation was performed on MCR, which, at the time of the simulation, was among the five largest computers in the world (see table1).

Table 1. Computing platform capabilities and statistical data for the GEODYN simulation of the BANEBERRY event.

MCR: Multiprogrammatic Capability Cluster	
No. of CPUs	2304
CPU Speed	2.4 GHz
Memory	2 Gb/CPU
Disk Space	225 Tb
Operating System	Linux

Statistical data for the Baneberry simulation	
Domain Size	~1 km
No. of cells	~40 million
No. of time steps	~3000
Simulated real time	~1 s
Simulation time	~40,000 CPU hours
Required storage	~3 Tb

The simulation helped establish a new capability to simulate underground test containment in 3D thus making it possible, for the first time, to accurately represent complex geologic features in the simulation. Comparison of the results of the study (see Fig. 1) with available data, and with the results of the previous 2D computational studies provided new insight into the cause of the baneberry containment failure.



(a) Pressure isosurface **(b)** Damage map

Figure 1. Pressure isosurface (a) and damage map from the 3D Baneberry simulation. The pressure isosurface plot illustrates the lack of spherical symmetry in the cavity region due to medium layering and nearby faults. The damage map shows three damaged regions (a weak clayey region in the vicinity of the working point, the faults, and a cone-shaped spalled region near surface ground zero) connected to one another, thereby forming a continuous damaged region that connects the WP to the surface fissure where the radioactive release was first detected just after the test.

Response of Underground Structures

We have recently used LDEC to perform simulations of unprecedented scale to evaluate the response of a deeply buried tunnel complex in a jointed geologic medium [2]. LDEC is a 3D massively parallel code developed at LLNL to simulate the response of underground tunnels and structures to dynamic loads. It represents the rock mass using a large number of polyhedral blocks that interact at their points of contact according to experimentally validated contact force laws. Facilities of interest may be hundreds of meters across within fractured rock masses where individual blocks may be much less than a meter in size. Even modeling a portion of such facilities requires millions of computational elements.

The simulation was performed on THUNDER, which at the time of the simulation was the second largest computer in the world. The simulation is the largest of its kind to date and included a detailed facility spanning approximately 50 m with multiple tunnels and junctions. The fracture spacing in the rock was 30 cm, resulting in a computational domain of ~8 million polyhedral blocks and ~100 million computational elements (see Table 2). The facility was subjected to loading from a near-surface explosion, resulting in collapsed portions of the tunnels (see Fig. 2).

Table 2. Computing platform capabilities and statistical data for the LDEC simulation of an underground tunnel complex.

THUNDER computing resource	
No. of CPUs	4008
CPU Speed	1.4 GHz Itanium 2
Memory	2 Gb/CPU
Disk Space	200TB
Operating System	Linux

Statistical data for the underground tunnel complex simulation	
Domain Size	~50m
No. of computational elements	~100 million
No. of time steps	~500,000
Simulated real time	~1s
Simulation time	~500,000 CPU hours
Required storage	~2 TB

This modeling approach represents a fundamental change in the way simulations of large scale underground structures are performed. By directly simulating the discrete, blocky nature of rock masses, LDEC takes a fundamental approach to simulating the behavior of these systems while limiting the number of empirically derived model features. This approach is analogous to the application of molecular dynamics where complicated results observed in simulations are emergent consequences of a large system with relatively simple, fundamental laws at work at the small scale.

Figure 2. Sequence of snapshots showing the progressive collapse of a section of the tunnel complex where an access drift intersect one of the main functional areas of the facility.

References

[1] Lomov, I., Antoun, T., Wagoner, J., and Rambo, J., "Three Dimensional Simulation of the Baneberry Nuclear Event," 13th APS Topical Conference on Shock Compression of Condensed Matter, (July 2003).

[2] Morris, J., “Thunder Science Runs: Simulation of Hard and Deeply Buried Targets using LDEC,” UCRL -PRES-206648 (2004).